Practical Guide to Support Vector Machines

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Outline

- Data Classification
- High-level Concepts of SVM
- Interpretation of SVM Model/Result
- Use Case Study

What does it mean to learn?

- Acquire new skills?

- Make predictions about the world?

Making predictions is fundamental to survival

Will that bear eat me?

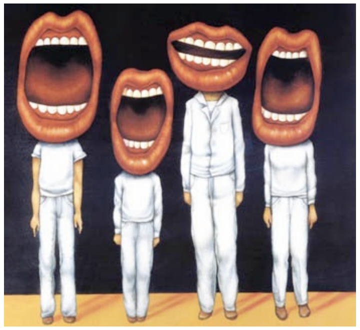
Is there water in that canyon?

Is that person a good mate?

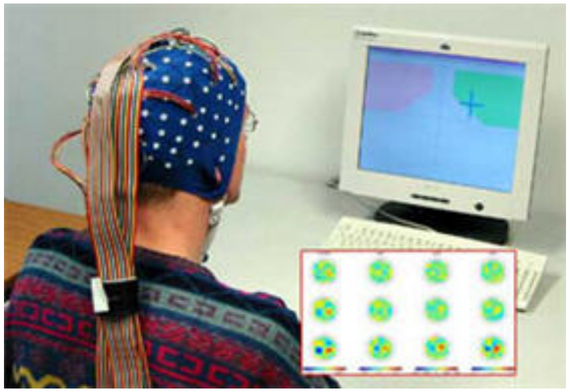
These are all examples of classification problems

Boot Camp Related

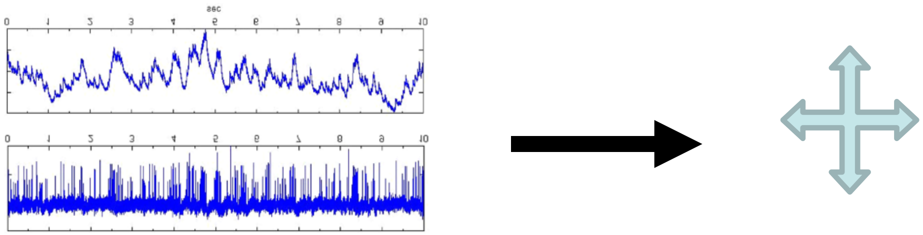
Motion classification



face recognition / speaker identification



Brain Computer Interface / Spikes Classification



Driver Fatigue Detection from Facial Expression

Data Classification

Sensor → Data Preprocessing (features) → Classifier → Prediction

Data Preprocessing

features

Classifier

SVM

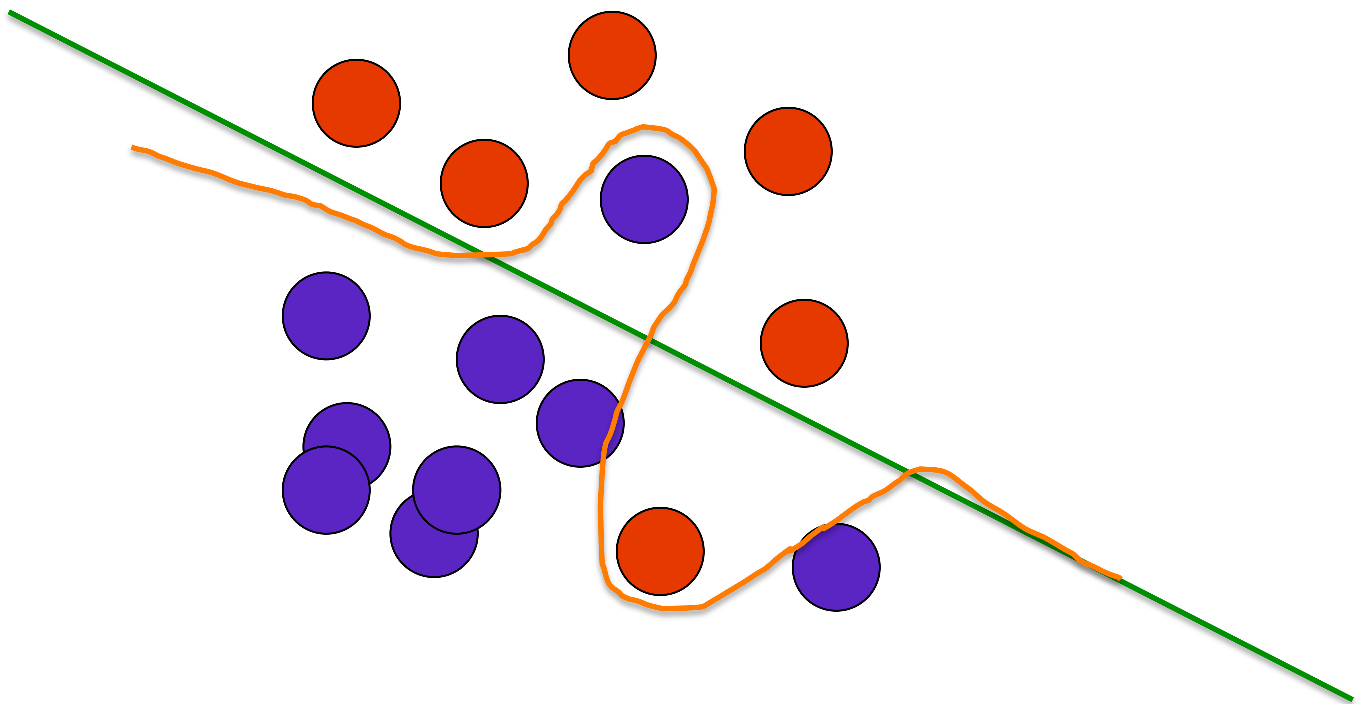
Adaboost

Neural Network

Prediction

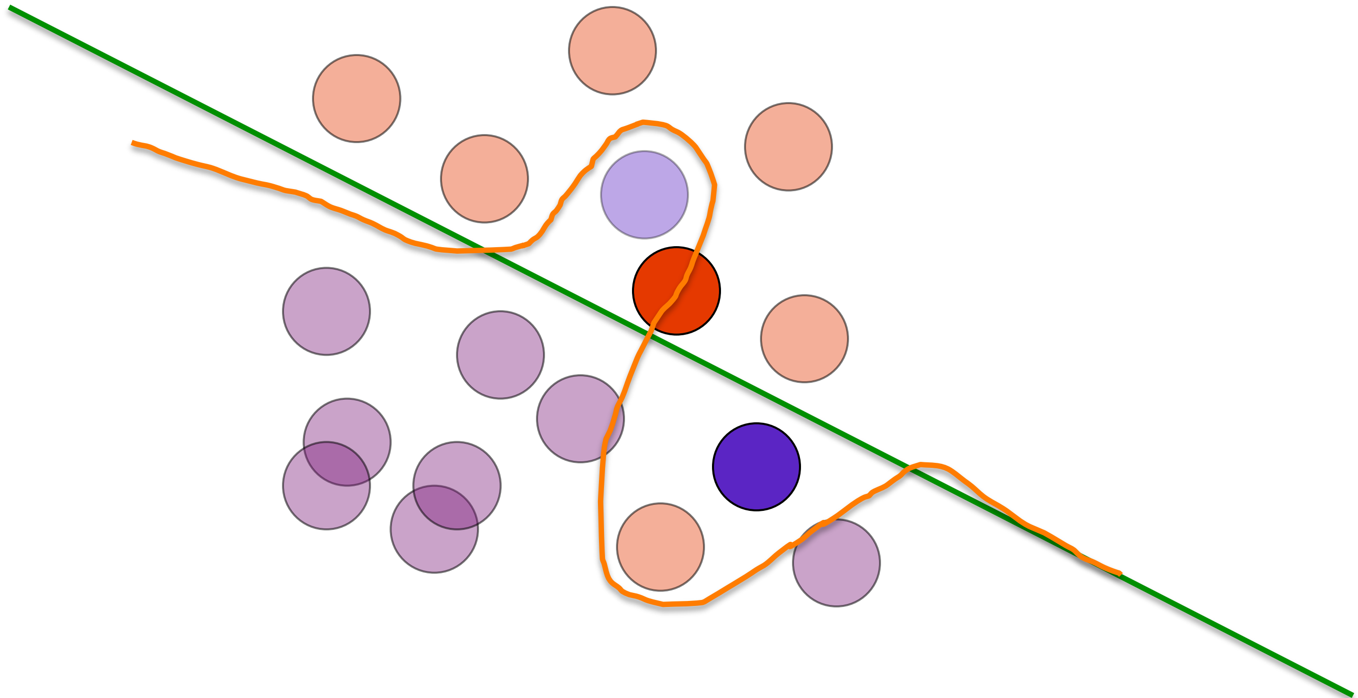
- Given training data (class labels known)
  Predicts test data (class labels unknown)
- Not just fitting → generalization

Generalization



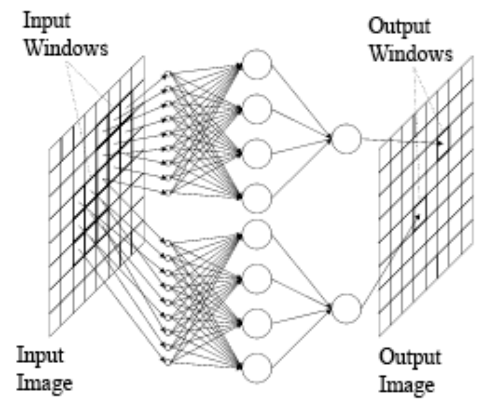
Many possible classification models
Which one generalize better ?

Generalization



Why SVM ? (my opinion)

- With careful data preprocessing, and properly use of SVM or NN → similar performance.



- SVM is easier to use properly.

- SVM provides a reasonable good baseline performance.

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A Simple Dilemma

Who do I invite to my birthday party?

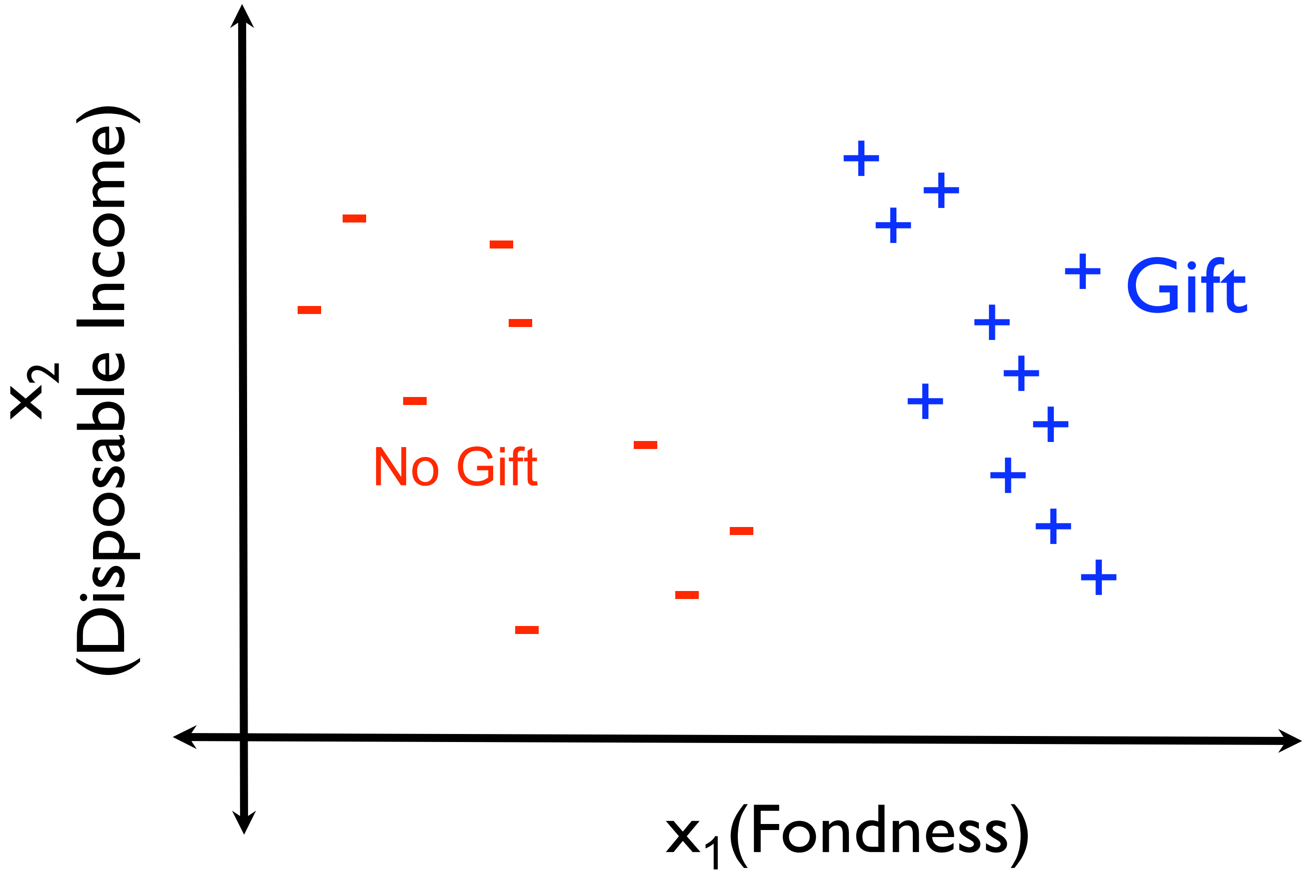
Problem Formulation

- training data as vectors: $\mathbf{x}_i$
- binary labels [+1, -1]

Name	Gift?	Income	Fondness
John	Yes	3k	3/5
Mary	No	5k	1/5

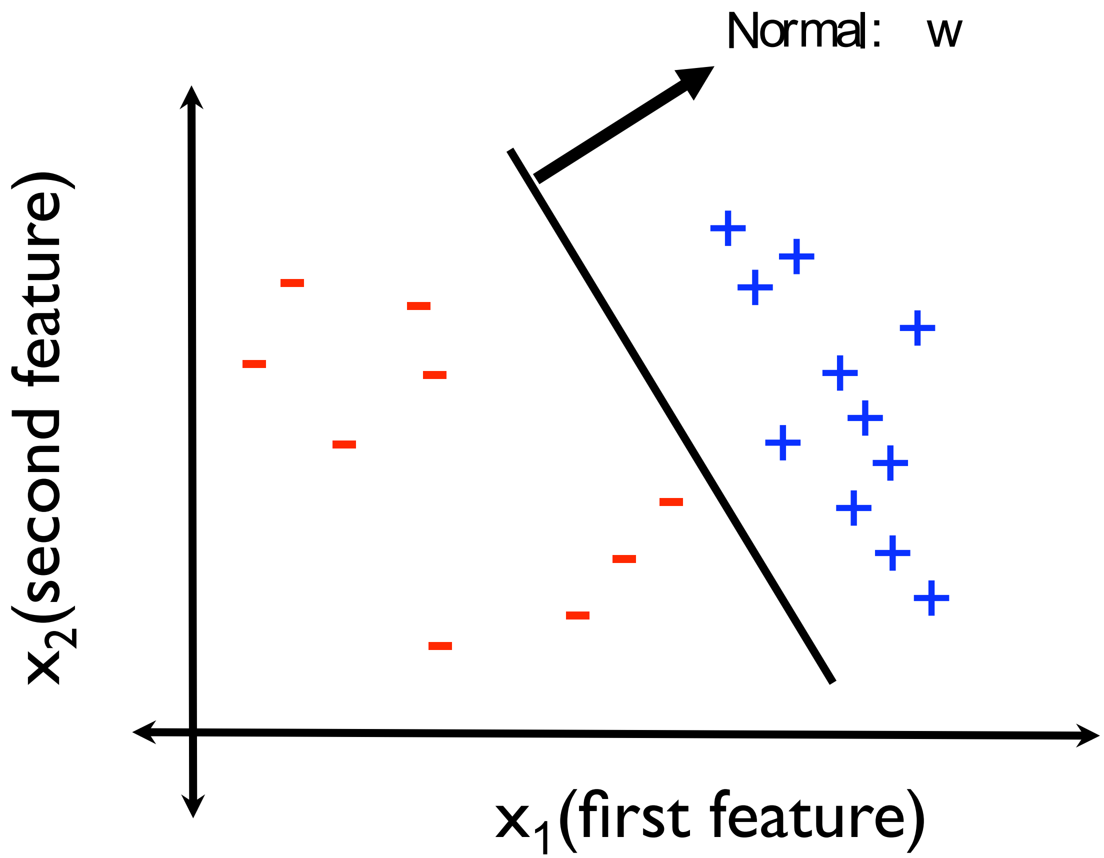
class	feature vector
y_1=+1	$\mathbf{x}_1$ = [3000, 0.6]
y_2= -1	$\mathbf{x}_2$ = [5000, 0.2]

Vector space



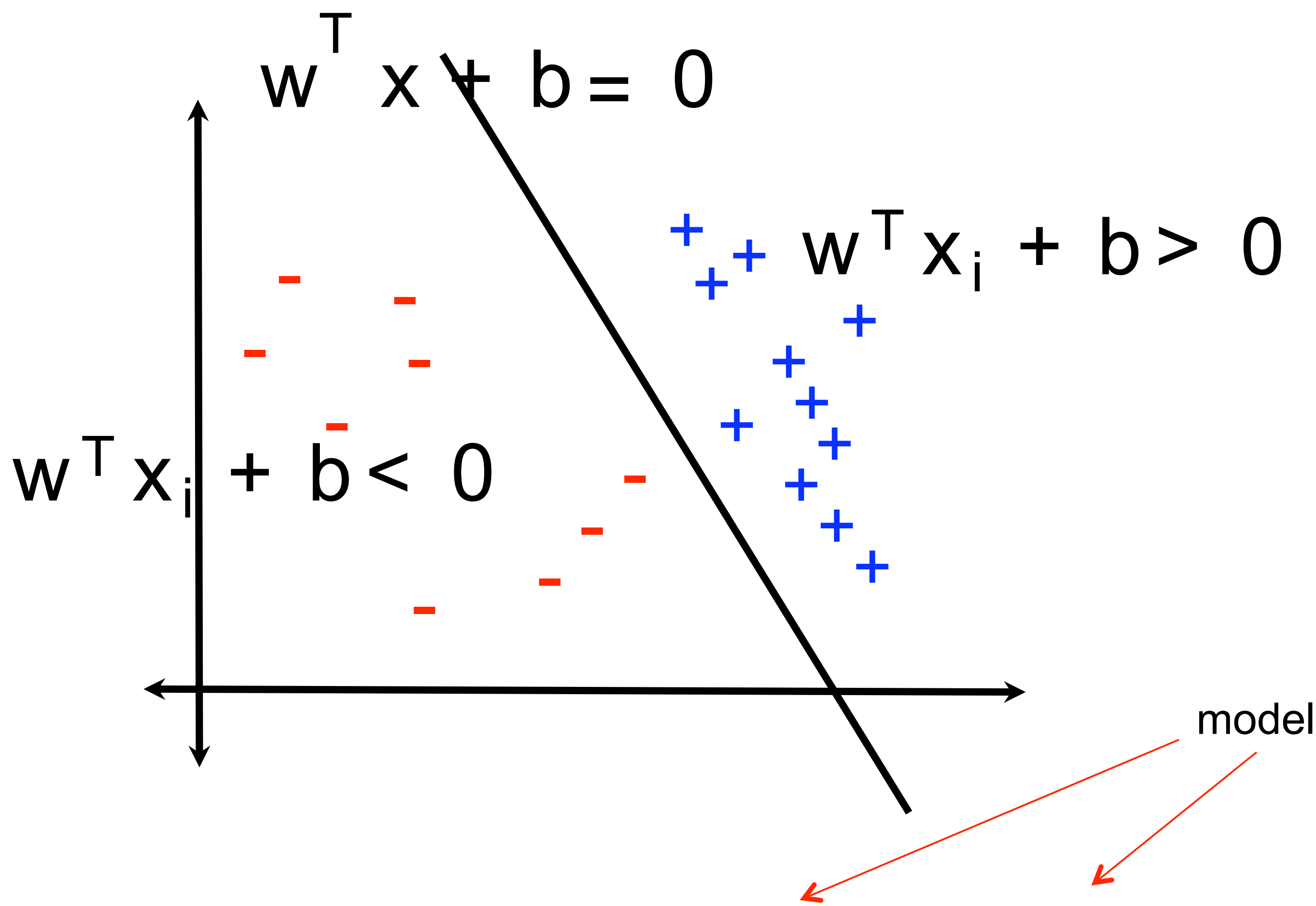
A Line

The line : $w^T x + b = 0$



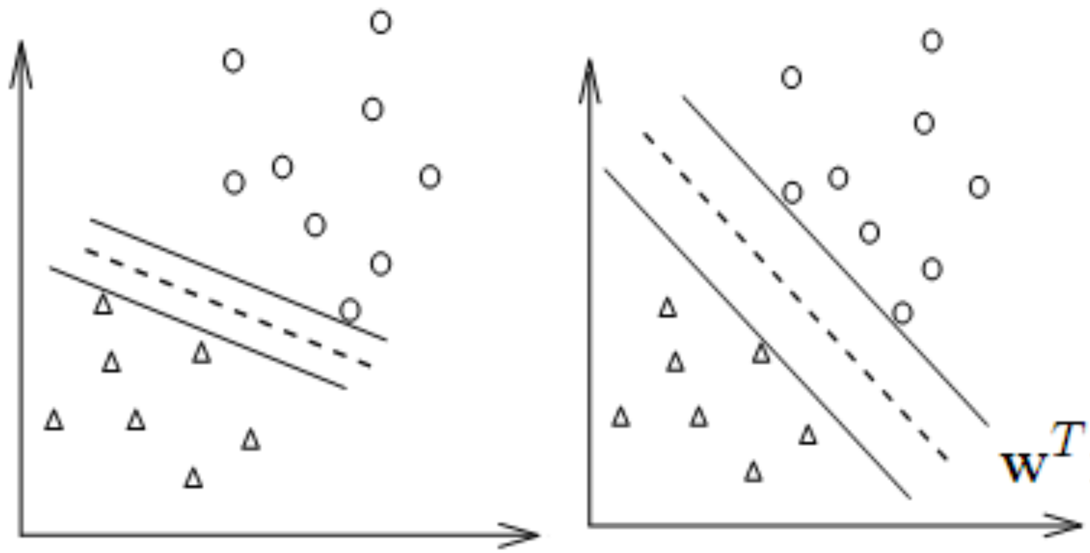
"Hyperplane" in high dimensional space

The inequalities and regions



Decision function $f(x) = \text{sign}(w^T x_{new} + b)$

Large Margin



$$\mathbf{w}^T\mathbf{x} + b = \begin{bmatrix} +1 \\ 0 \\ -1 \end{bmatrix}$$

A separating hyperplane: $\mathbf{w}^T\mathbf{x} + b = 0$

$$(\mathbf{w}^T\mathbf{x}_i) + b > 0 \quad \text{if } y_i = 1$$
$$(\mathbf{w}^T\mathbf{x}_i) + b < 0 \quad \text{if } y_i = -1$$

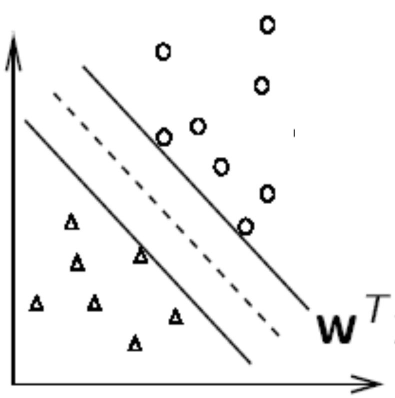
Maximal Margin

Distance between $\mathbf{w}^T\mathbf{x} + b = 1$ and -1:

$$2/\|\mathbf{w}\| = 2/\sqrt{\mathbf{w}^T\mathbf{w}}$$

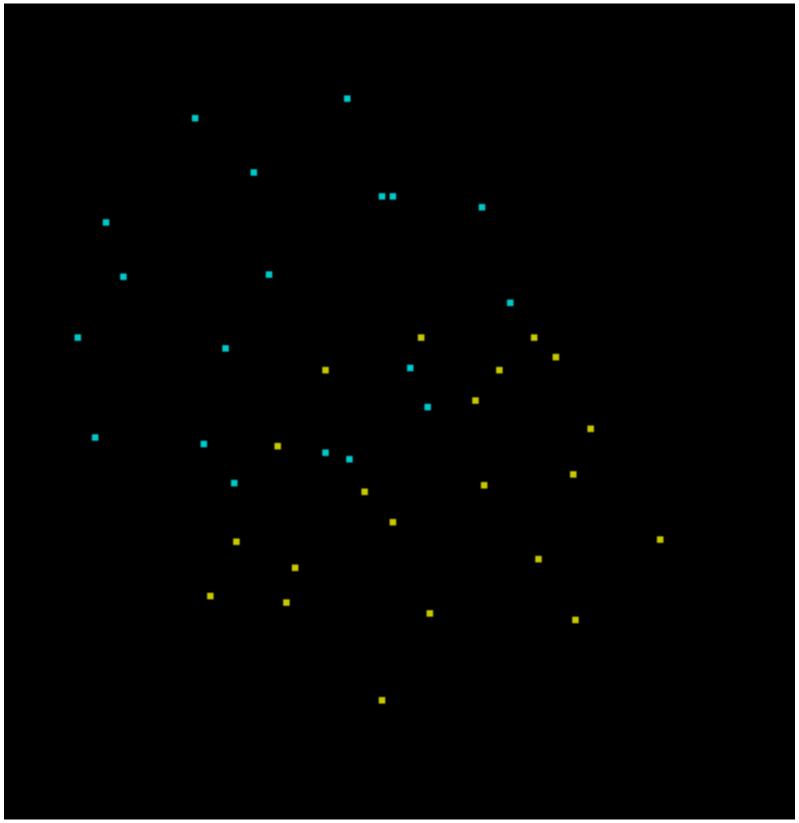
$$\max 2/\|\mathbf{w}\| \equiv \min \mathbf{w}^T\mathbf{w}/2$$

$$\begin{aligned} \min_{\mathbf{w},b} \quad & \frac{1}{2}\mathbf{w}^T\mathbf{w} \\ \text{subject to} \quad & y_i((\mathbf{w}^T\mathbf{x}_i) + b) \geq 1, \\ & i = 1, \dots, l. \end{aligned}$$

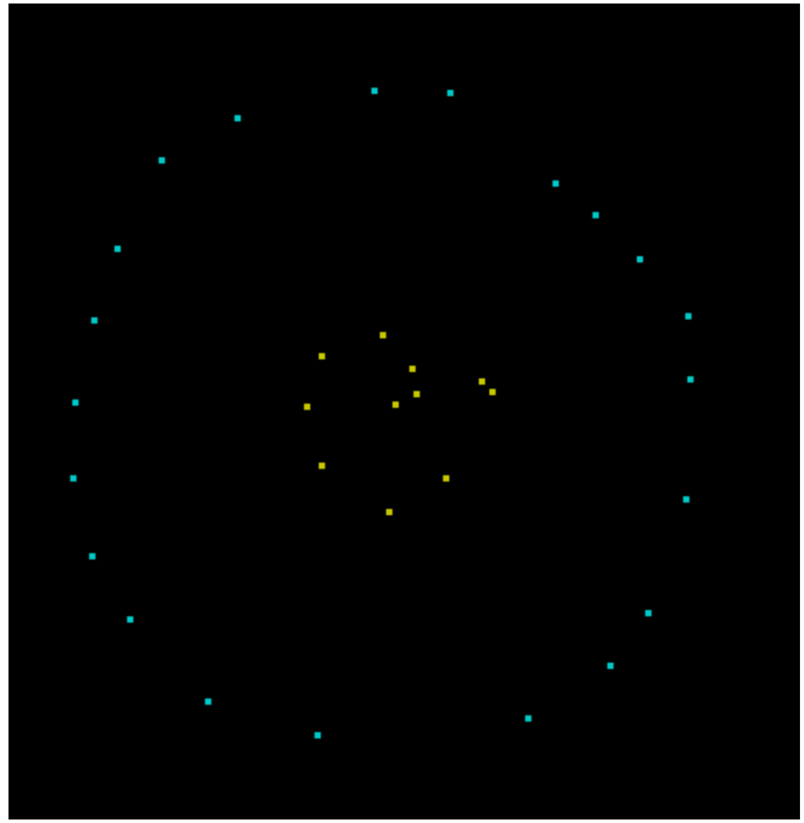


$$\mathbf{w}^T\mathbf{x} + b = \begin{bmatrix} +1 \\ 0 \\ -1 \end{bmatrix}$$

Data not linearly separable



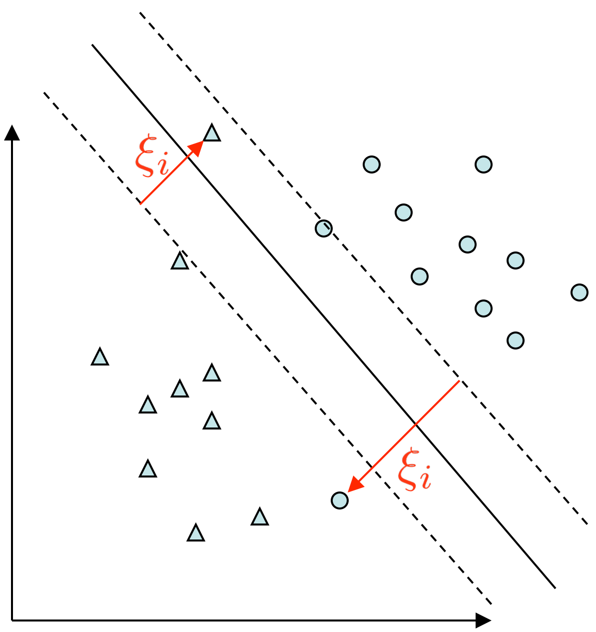
Case 1



Case 2

Trick 1: Soft-Margin

These points are usually outliers. The hyperplane should not bias too much.



Penalty of violating data

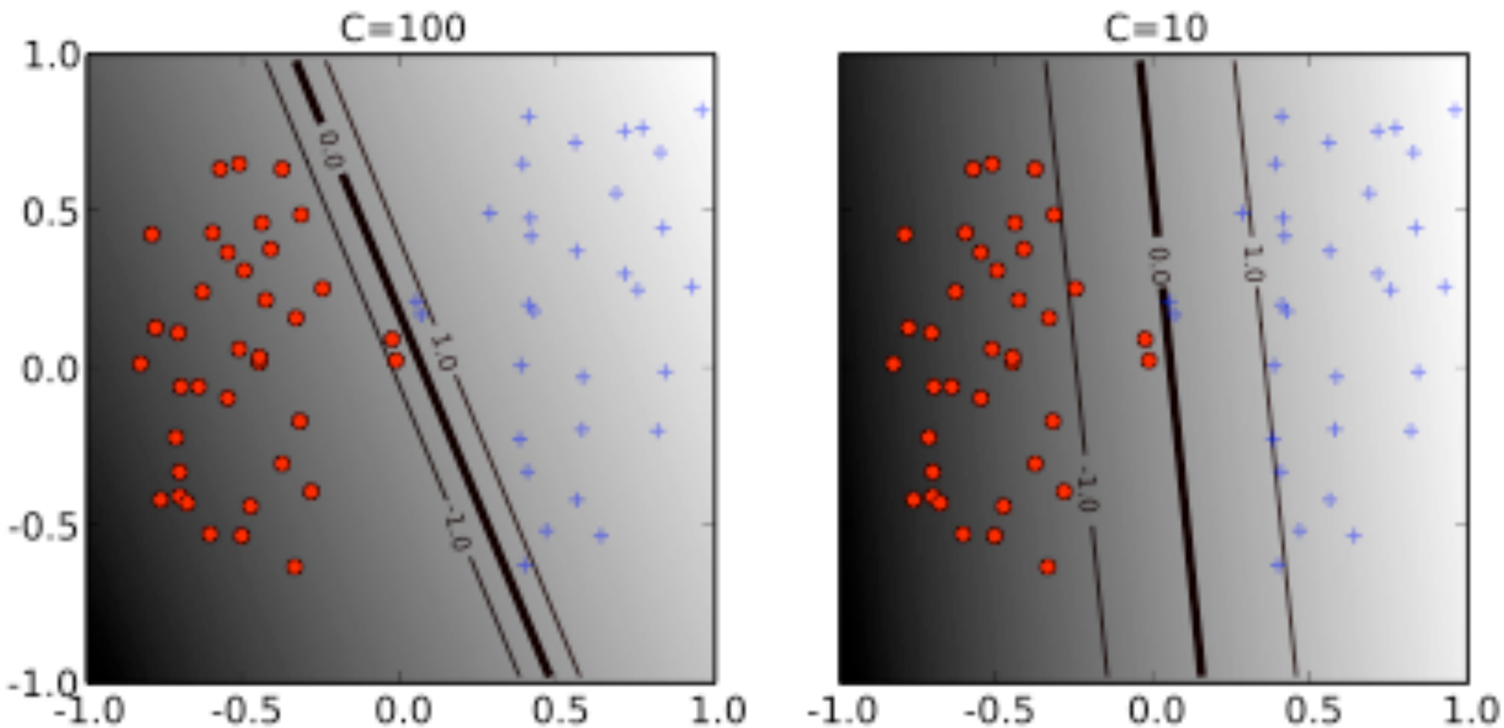
$$\min_{w,b} \quad \frac{1}{2}w^T w + C\sum_i \xi_i$$

$$\text{subject to} \quad y_i(w^T x_i + b) \geq 1 - \xi_i$$

$$\xi \geq 0$$

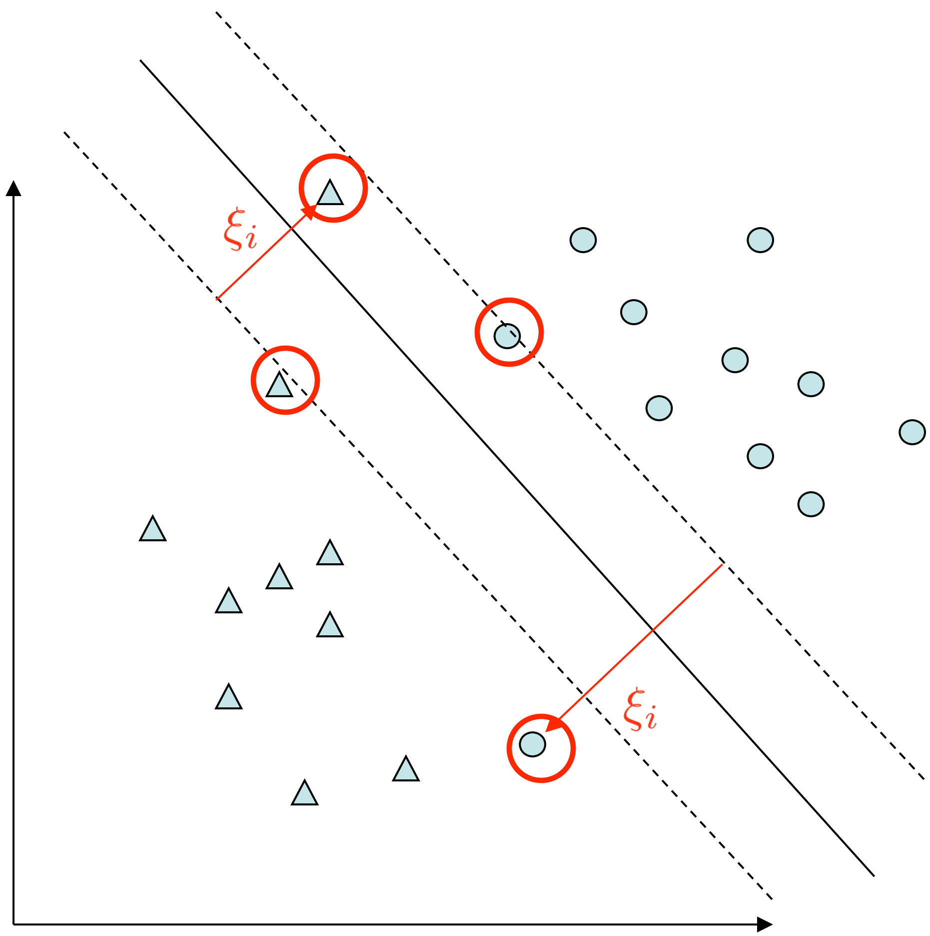
C: large penalty parameter, most ξ_i are zero

Soft-margin



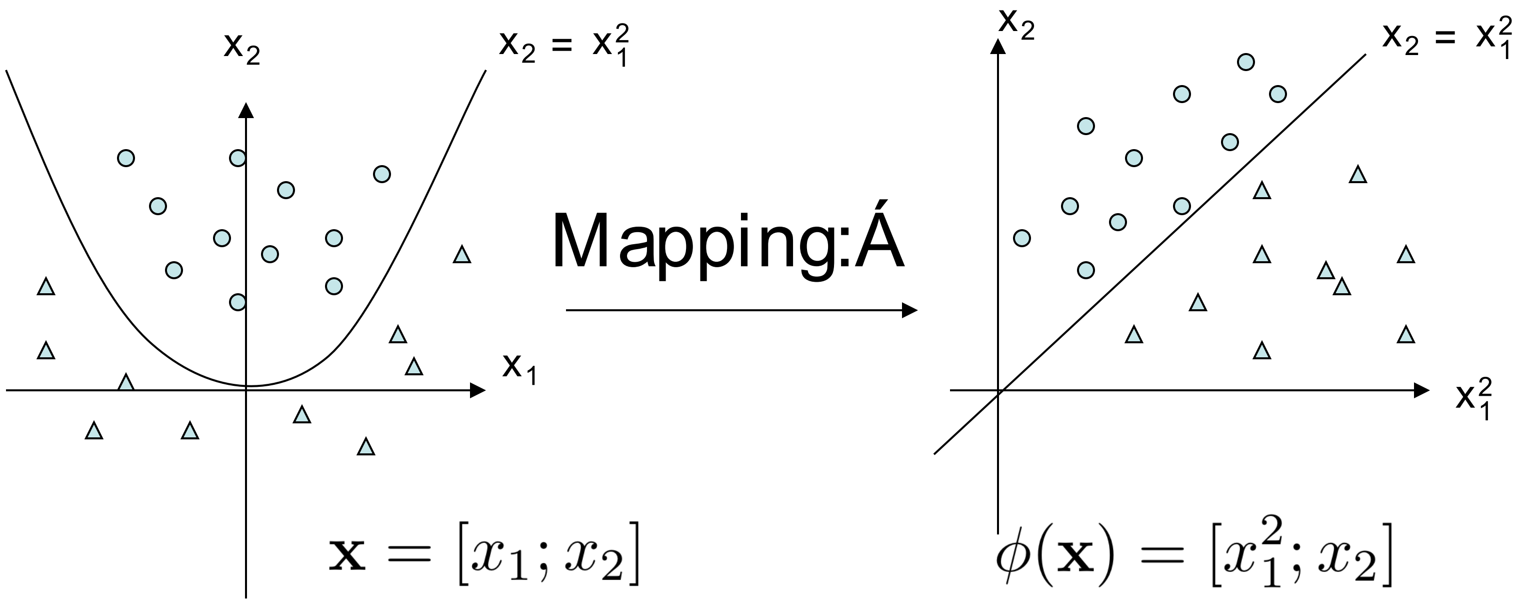
[Ben-Hur & Weston 2005]

Support vectors



More important data that support (define) the hyperplane

Trick2: Map to Higher Dimension



$$\mathbf{x} = [x_1; x_2] \qquad \phi(\mathbf{x}) = [x_1^2; x_2]$$

$$\min_{w,b} \quad \frac{1}{2} w^T w + C \sum_i \xi_i$$

$$\text{subject to} \quad y_i(w^T \phi(x)_i + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

Mapping to Infinite Dimension

- Is it possible to create a universal mapping ?
- What if we can map to infinite dimension ? Every problem is separable!

- Consider "Radial Basis Function (RBF)":

$$\phi(x) = e^{-\gamma x^2}[1, \sqrt{\frac{2\gamma}{1!}}x, \sqrt{\frac{(2\gamma)^2}{2!}}x^2, \sqrt{\frac{(2\gamma)^3}{3!}}x^3, \cdots]^T$$

- $\phi(\mathbf{x})^T\phi(\mathbf{y}) \;=\; e^{-\gamma\|x_i - x_j\|^2}$ =Kernel(x,y)

w : infinite number of variables!

$$\begin{aligned} \min_{w,b} \quad & \frac{1}{2}w^T w + C\sum_i \xi_i \\ \text{subject to} \quad & y_i(w^T\phi(x)_i + b) \geq 1 - \xi_i \\ & \xi_i \geq 0 \end{aligned}$$

Dual Problem

- Primal

$$\min_{w,b} \quad \frac{1}{2}w^T w + C\sum_i \xi_i$$

$$\text{s.t.} \quad y_i(w^T\phi(x)_i + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

- Dual

$$\min_{\alpha} \quad \frac{1}{2}\alpha^T Q\alpha - \sum_i \alpha_i$$

$$\text{where} \quad Q_{ij} = y_i y_j \underline{\phi(x_i)^T\phi(x_j)}$$

$$\text{s.t.} \quad \sum \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C$$

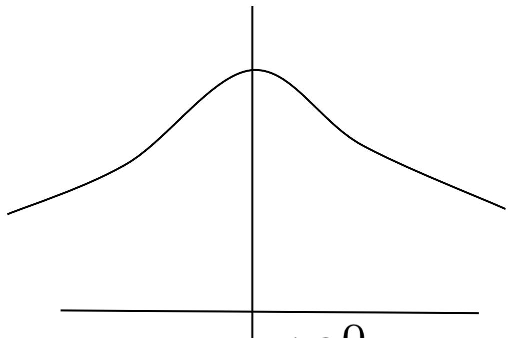
$$\phi(x_i)^T\phi(x_j) = e^{\gamma|x_i - x_j|}$$

finite calculation

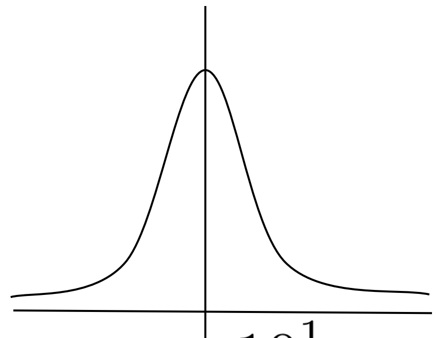
$$\mathbf{w} = \sum_{i=1}^{l} \alpha_i y_i \phi(\mathbf{x}_i)$$

Gaussian/RBF Kernel

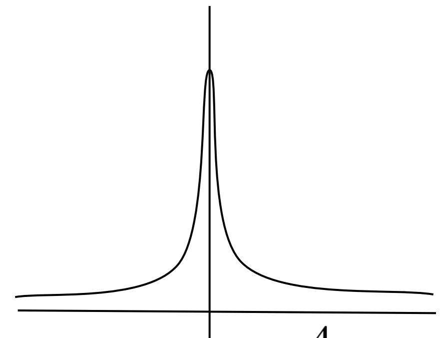
$$\phi(x_i)^T\phi(x_j) = e^{-\gamma|x_i - x_j|} = e^{-dist(x_i,x_j)} = \text{similarity}(x_i, x_j)$$



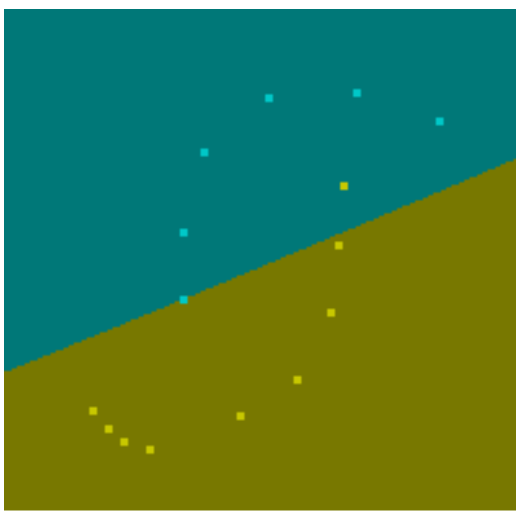
$\gamma = 10^0$



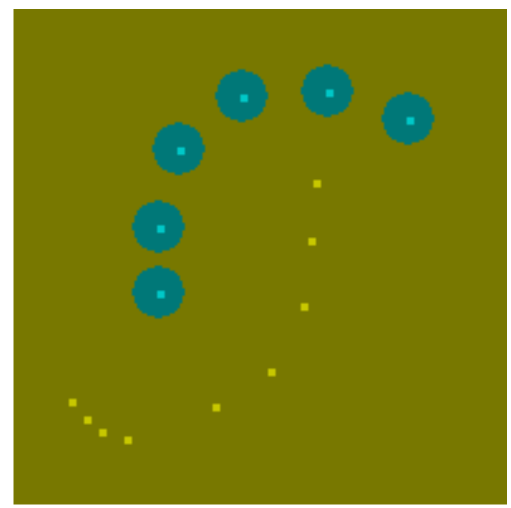
$\gamma = 10^1$



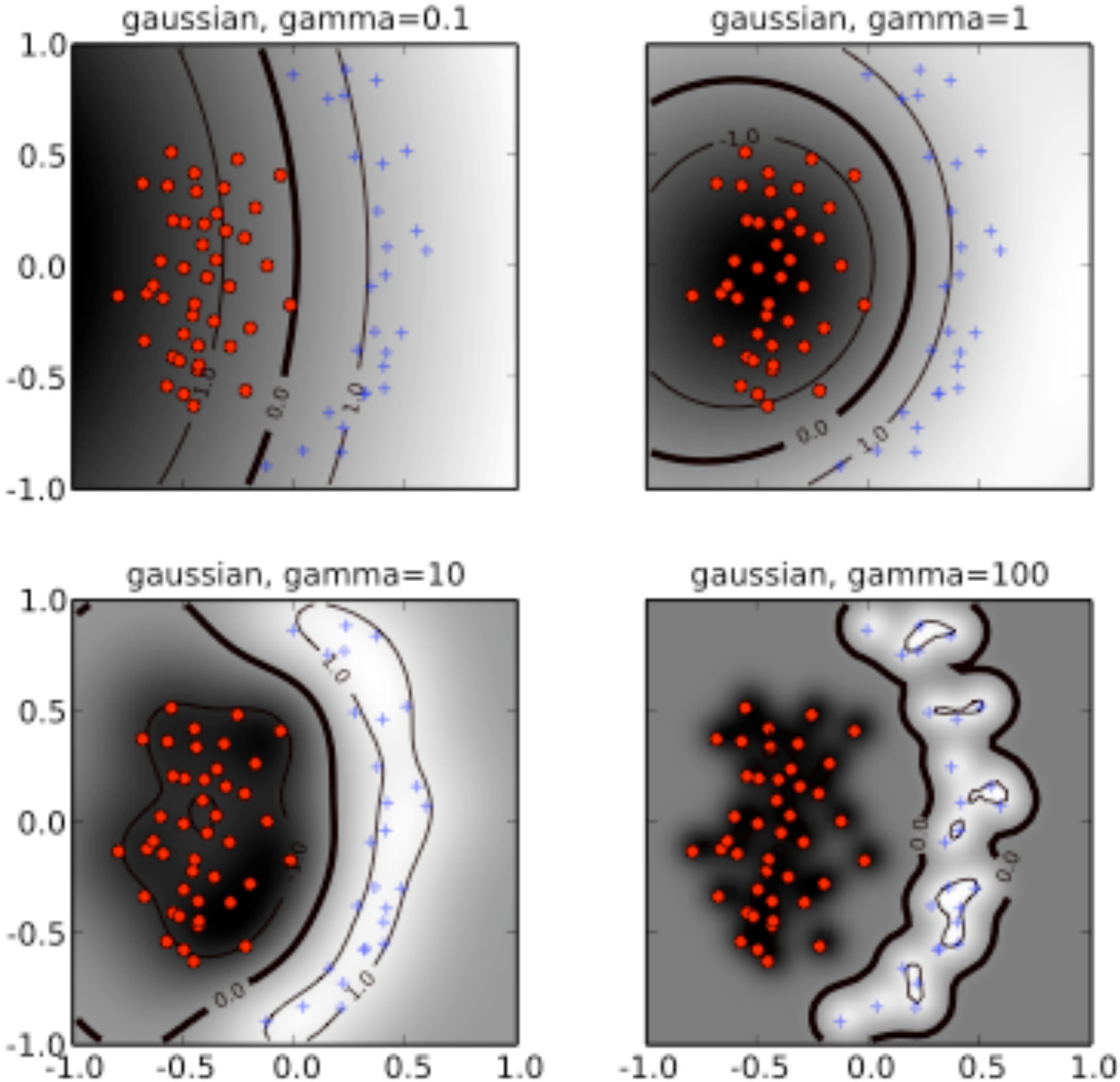
$\gamma = 10^4$



~ linear kernel

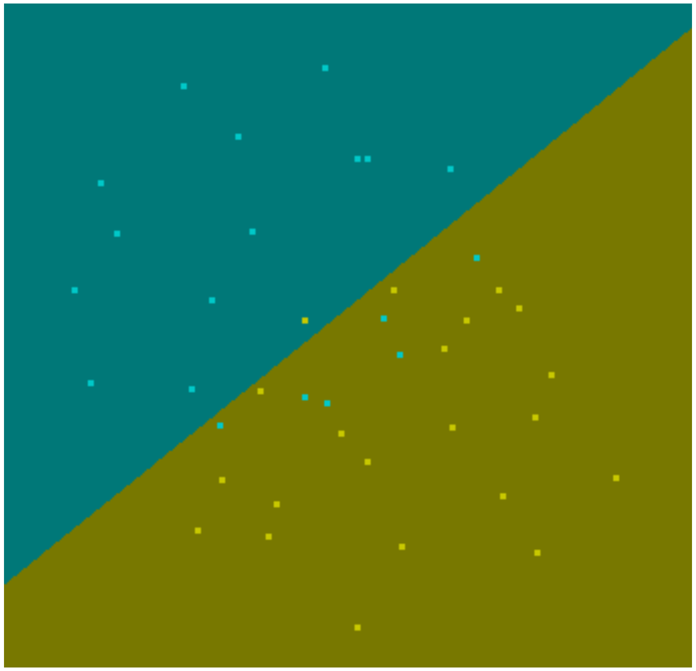


Overfitting
nearest neighbor?

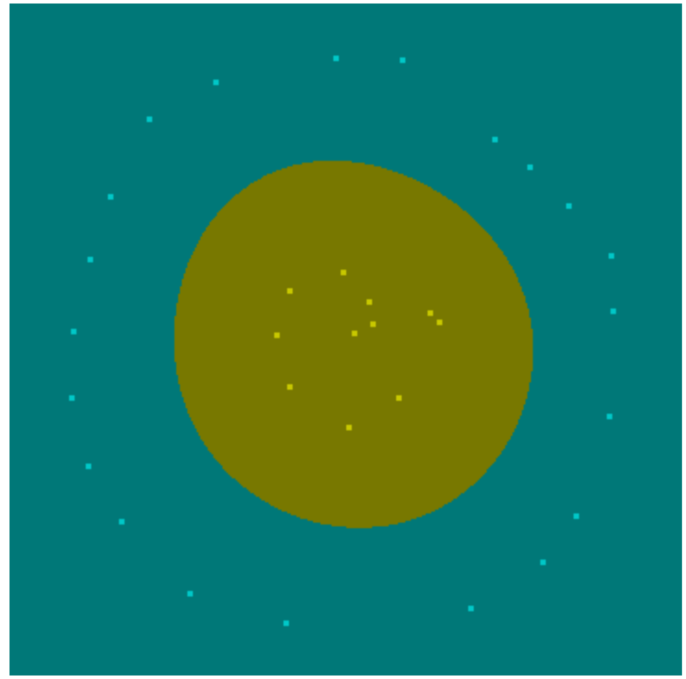


[Ben-Hur & Weston 2005]

Recap



Soft-ness



Nonlinearity

$$\min_{w,b} \quad \frac{1}{2} w^T w + C \sum_i \xi_i$$

$$\text{s.t.} \quad y_i(w^T \phi(x)_i + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

$$\phi(x_i)^T \phi(x_j) = e^{-\gamma |x_i - x_j|}$$

Checkout the SVMToy

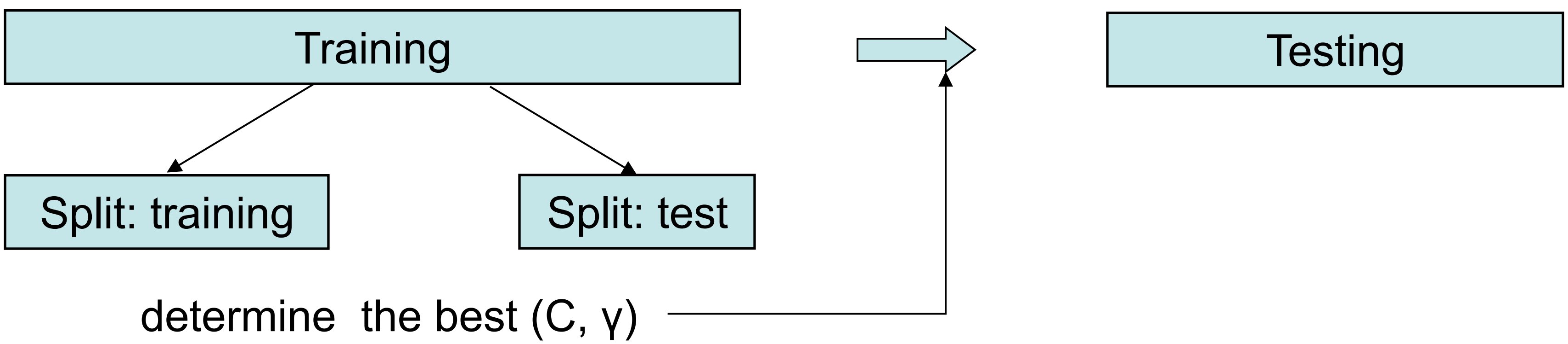
- http://www.csie.ntu.edu.tw/~cjlin/libsvm/

- -c (cost control softness of the margin/#SV)
- -g (gamma controls the curvature of the hyperplane)

Cross Validation

•What is the best (C, γ) ? → Date dependent
•Need to be determined by "testing performance"

•Split training data into pseudo "training, testing" sets



•Exhausted grid search for best (C, γ)

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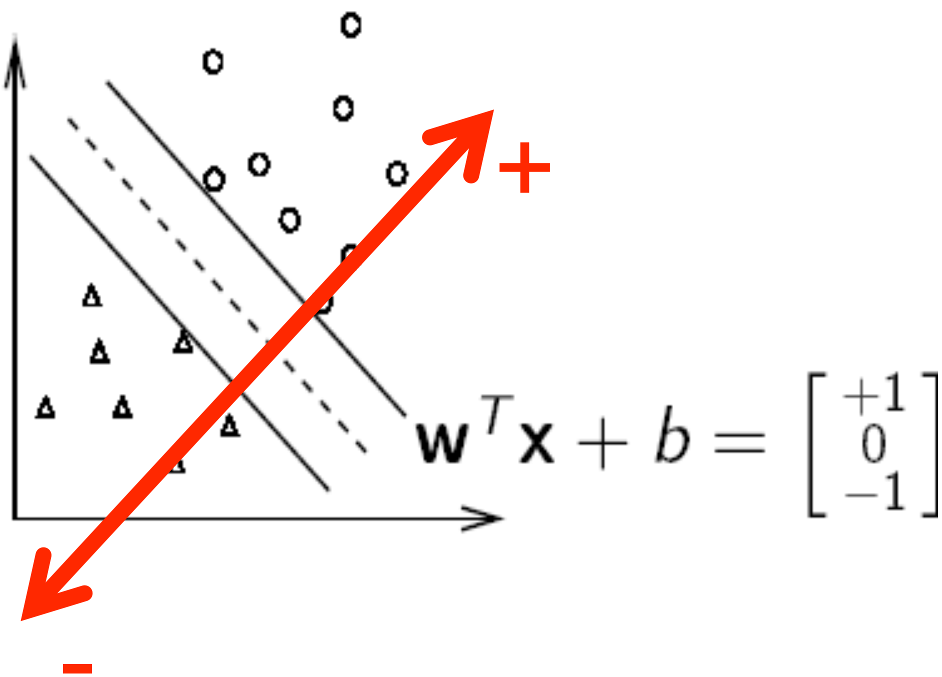
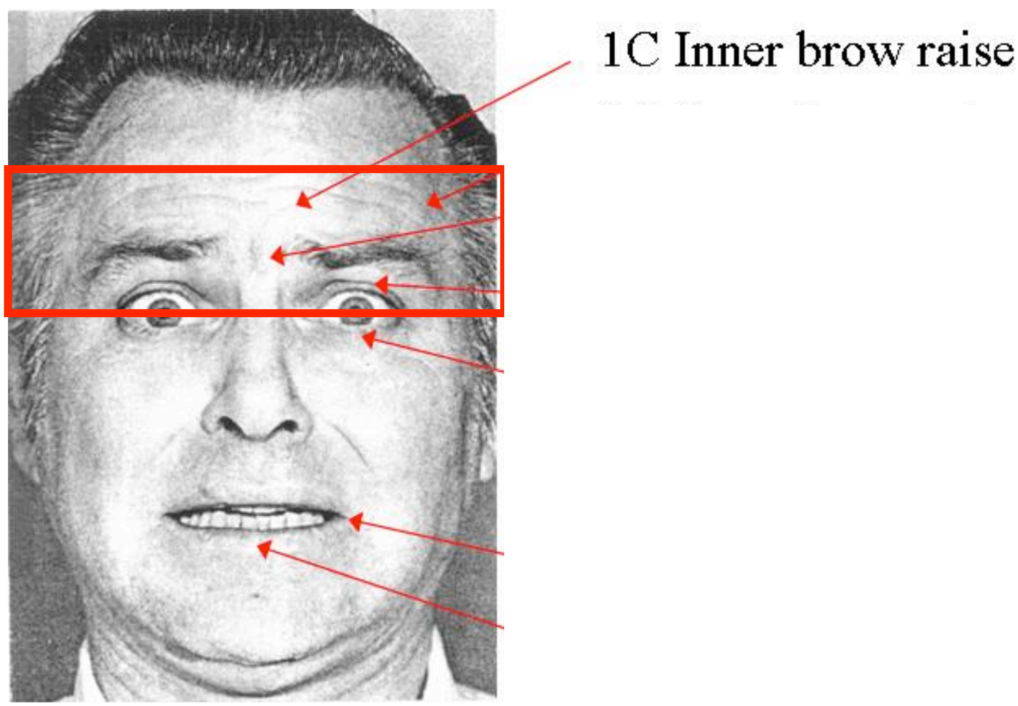
(1)Decision value as strength

Decision function $f(x) = \text{sign}(w^T x_{new} + b)$



Facial Movement Classification

- Classes: brow up(+) or down(-)
- Features: pixels of Gabor filtered image

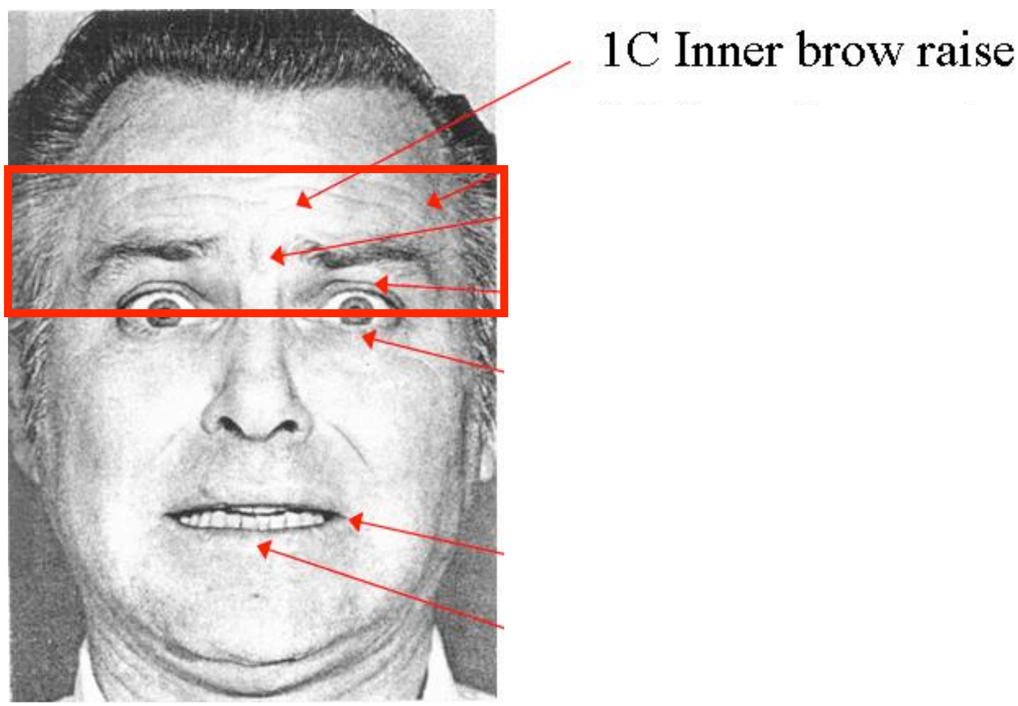


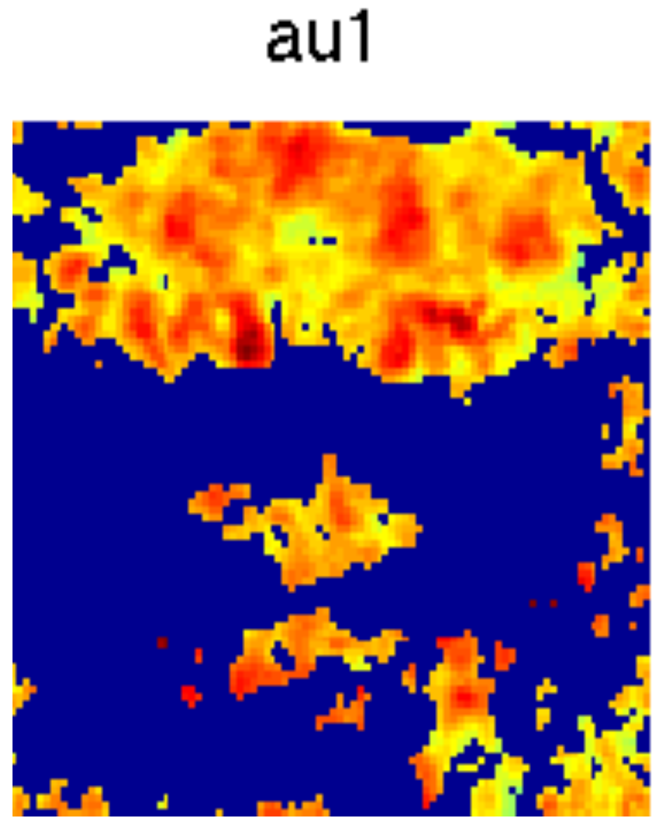
Decision value as strength

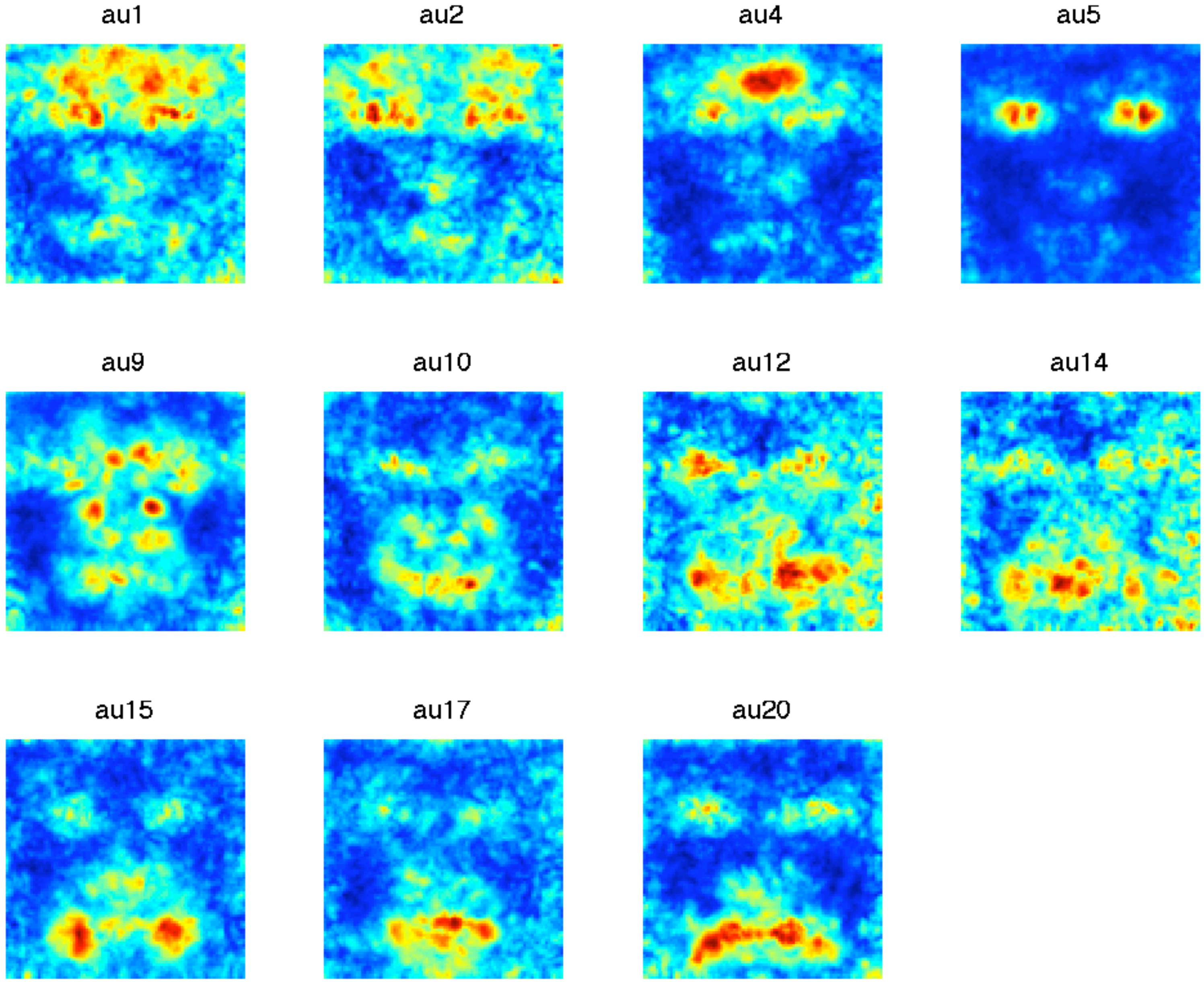
Probability estimates from decision values also available

(2)Weight as feature importance

- Magnitude of weight : feature importance
- Similar to regression






au1
au2
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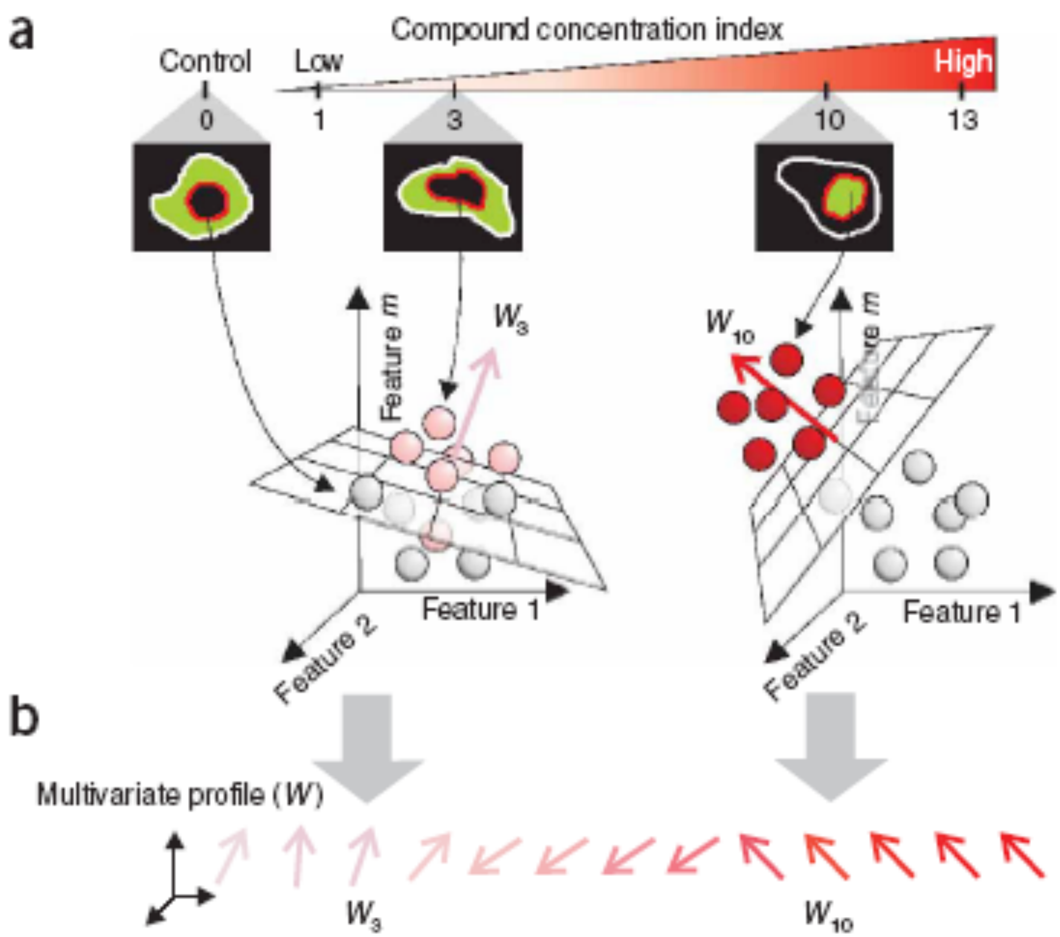
au20

(3)Weights as profiles



Fluorescent image of cells of various **dosage** of certain drug

Various image-based features

Clustering the weights shows the primal and secondary effect of the drug

Lit-Hsin Loo, Lani F Wu & Steven J Altschuler

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The Software

- SVM requires an constraint quadratic optimization solver
  →not easy to implement.
- Off-the-shelf Software
  - libsvm by Chih-Jen Lin et. al.
  - svm^{light} by Thorsten Joachims
- Incorporated into many ML software
  - matlab / pyML / R…

Beginners may…

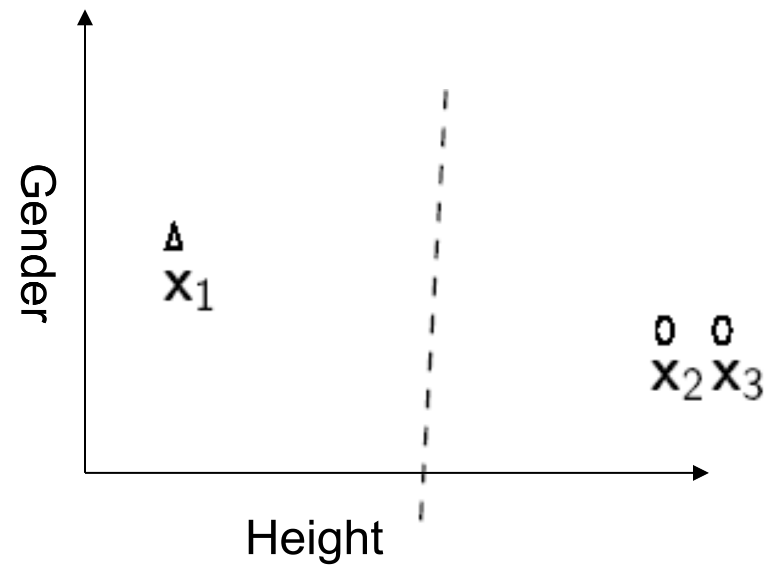
1. Convert their data into the format of a SVM software.
2. May not conduct scaling
3. Randomly try few parameters and without cross validation
4. Good result on training data, but poor in testing.

Data scaling

Without scaling

–feature of large dynamic range may dominate separating hyperplane.

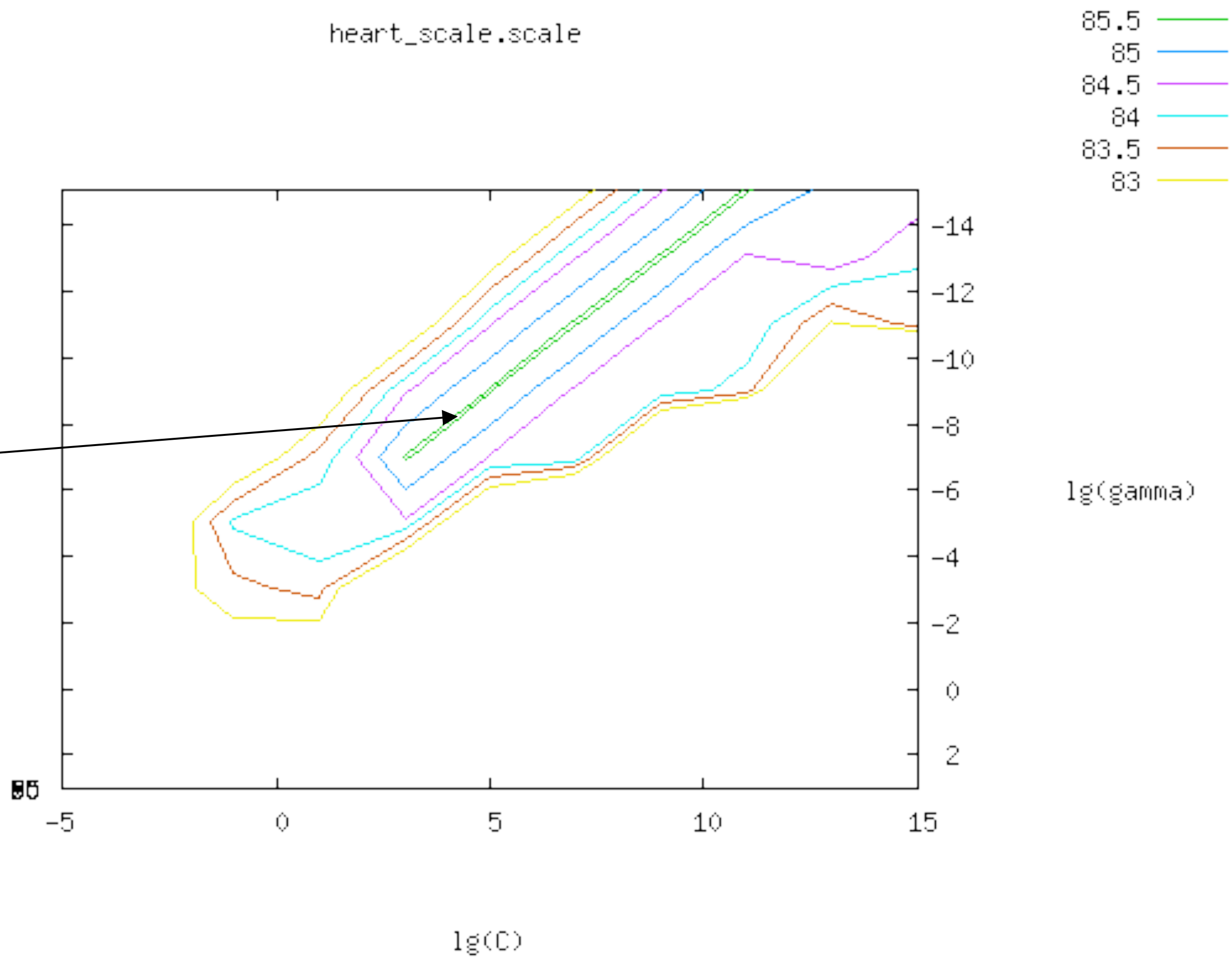
label	X	Height	Gender
y1=0	x1	150	2
y2=1	x2	180	1
y3=1	x3	185	1



Parameter Selection

Contour of cross validation accuracy.

Good area



User case : Astroparticle scientist

- User:
  I am using libsvm in a astroparticle physics application .. First, let me congratulate you to a really easy to use and nice package. Unfortunately, it gives me astonishingly bad test results...
- OK. Please send us your data
  We are able to get 97% test accuracy. Is that good enough for you ?
- User:
  You earned a copy of my PhD thesis

Dynamic Range Mismatch

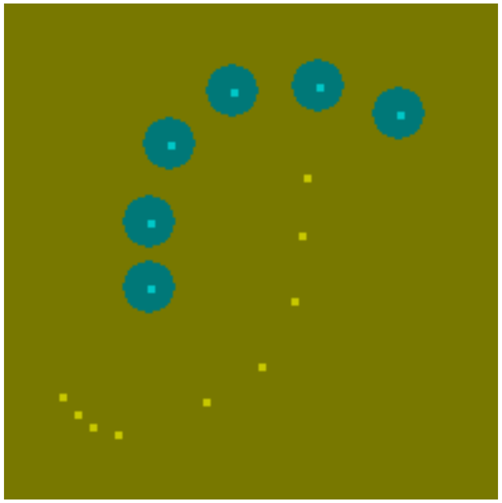
- A problem from astroparticle physics

<label> <index>:<value> <index>:<value> …
1 1:2.6173e+01 2:5.88670e+01 3:-1.89469e-01 4:1.25122e+02
1 1:5.7073e+01 2:2.21404e+02 3:8.60795e-02 4:1.22911e+02
1 1:1.7259e+01 2:1.73436e+02 3:-1.29805e-01 4:1.25031e+02
1 1:2.1779e+01 2:1.24953e+02 3:1.53885e-01 4:1.52715e+02
1 1:9.1339e+01 2:2.93569e+02 3:1.42391e-01 4:1.60540e+02
1 1:5.5375e+01 2:1.79222e+02 3:1.65495e-01 4:1.11227e+02
1 1:2.9562e+01 2:1.91357e+02 3:9.90143e-02 4:1.03407e+02

- #Training set 3,089 and #testing set 4,000
- Large dynamic range of some features.

Overfitting

- Training
  $./svm-train train.1   (default parameter used)
  optimization finished, #iter = 6131
  nSV = 3053, nBSV = 724
  Total nSV = 3053



- Training Accuracy
  $./svm-predict train.1 train.1.model o
  Accuracy = 99.7734% (3082/3089)

- Testing Accuracy
  $./svm-predict test.1 train.1.model test.1.out
  Accuracy = 66.925% (2677/4000)
  nSV and nBSV: number of SVs and bounded SVs (i = C).
  Without scaling. One feature may dominant the value overfitting

•3053/3089 training data become support vector→Overfitting
•Training accuracy high, but low testing accuracy → Overfitting

Suggested Procedure

- Data pre-scaling
  - scale range [0 1] or unit variance
- Using (default) Gaussian(RBF) kernel
- Use cross-validation to find the best parameter (C,γ)
- Train your model with best parameter
- Test!

All above done automatically in "easy.py" script provided with libsvm.

Large Scale SVM

- (#training data >> #feature) and linear kernel
  - Use primal solvers (eg. liblinear)
- To approximated result in short time
  - Allow inaccurate stopping condition
    svm-train –e 0.01
  - Use stochastic gradient descent solvers

  - 24

Resources

- LIBSVM: http://www.csie.ntu.edu.tw/~cjlin/libsvm
- LIBSVM Tools: http://www.csie.ntu.edu.tw/~cjlin/libsvmtools
- Kernel Machines Forum: http://www.kernel-machines.org
- Hsu, Chang, and Lin: A Practical Guide to Suppor t Vector Classification
- my email: tfwu@ucsd.edu

- Acknowledgement
  - Many slides from Dr. Chih-Jen Lin , NTU